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New ENDF/B-VII.0 evaluations of neutron cross sections for 32 fission products

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New ENDF/B-VII.0 evaluations of neutron cross sections for 32 fission products

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Abstract. Neutron cross sections for fission products play important role not only in the design of extended burn-up core and fast reactors, but also in the study of the backend fuel cycle and the criticality analysis of spent fuel. New evaluations in both the resonance and fast neutron regions were performed by the KAERI-BNL collaboration for 32 fission products. Theses were ^{95}Mo, ^{101}Ru, ^{103}Rh, ^{105}Pd, ^{109}Ag, ^{131}Xe, ^{133}Cs, ^{141}Pr, and complete isotope chains of $^{142-148,150}$Nd, $^{144,147,148-154}$Sm, and $^{156,158,160-164}$Dy. The evaluations cover a large amount of reaction channels, including all those needed for neutronics calculations. Also, they cover the entire energy range, from 10^{-5} eV to 20 MeV, including the thermal, resolved, and unresolved resonance regions, and the fast neutron region.

1 Introduction

Neutron induced nuclear data for 32 fission products were evaluated under the KAERI-BNL collaboration. All evaluations were adopted by the new U.S. Evaluated Nuclear Data Library, ENDF/B-VII.0, released in December 2006 [1]. The list of fission products consists of the priority materials for several applications, extended to cover complete isotopic chains for three elements. Table 1 shows the full list of fission products evaluated in this work.

Table 1. Fission products evaluated in this work. Shown in **bold** are priority materials.

	Nuclides
Individual nuclides	^{95}**Mo,** ^{101} **Ru,** ^{103}**Rh,** ^{105}**Pd,** ^{109}**Ag,** ^{131}**Xe,** ^{133}**Cs,** ^{141}**Pr**
Neodymium	$^{142,\mathbf{143},144,\mathbf{145},146,147,148,150}$**Nd**
Samarium	$^{144,\mathbf{147},148,\mathbf{149},\mathbf{150},\mathbf{151},\mathbf{152},153,154}$**Sm**
Dysprosium	^{156,158,160,161,162,163,164}Dy

Our evaluation methodology covers both the low energy region and the fast neutron region. In the low energy region, our evaluations are based on the latest data published in the Atlas of Neutron Resonances [2]. This resource was used to infer both the thermal values and the resolved resonance parameters that were validated against the capture resonance integrals. In the unresolved resonance region we performed the additional evaluation by using the averages of the resolved resonances and adjusting them to the experimental data.

In the fast neutron region, our evaluations are based on the nuclear reaction model code EMPIRE-2.19 [3] validated against the experimental data. EMPIRE is the modular system of codes consisting of many nuclear reaction models, including the spherical and deformed optical model, Hauser-Feshbach theory with the width fluctuation correction and complete γ-ray emission cascade, DWBA, Multi-step Direct and Multi-step Compound models, and several versions of the phenomenological preequilibrium models. The code is equipped with a powerful GUI, allowing an easy access to support libraries such as RIPL-2 [4] and CSISRS/EXFOR [5], the graphical package, as well the utility codes for formatting and checking.

In general, we used the Reference Input Parameter Library, RIPL-2, for the initial set model parameters. These parameters were properly adjusted to reproduce the available experimental data taken from the CSISRS/EXFOR library.

2 Atlas-EMPIRE Evaluation Methodology

Our evaluations are based on the Atlas-EMPIRE methodology developed over several recent years by the National Nuclear Data Center, BNL with several external collaborators. This methodology covers both the low-energy region (thermal energy, resolved resonances, unresolved resonances) and the fast neutron energy region. In the the low-energy region, the evaluations are based on Mughabghab's new Atlas of Neutron Resonances. In the fast-neutron energy region, the evaluations are based on the nuclear reaction model code system EMPIRE developed by Herman *et al.*.

2.1 Low-energy region

A statistical analysis of neutron resonances was used by S. Mughabghab, BNL, to produce the well known BNL-325. Its 5^{th} edition was published in 2006 as the "Atlas of Neutron Resonances: Resonance Parameters and Thermal Cross Sections, Z = 1 - 100" [2], representing a considerable update to the 1981 [6] and 1984 [7] editions of BNL-325. These latest thermal values and resonance parameters provided a basis for more than 150 new evaluations included in ENDF/B-VII.0, with the resolved and unresolved resonance parameters adopted from Ref. [2]. Figure 1 shows the evaluated capture cross sections for ^{133}Cs in thermal and resolved resonance

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regions and compares them with the available experimental data.

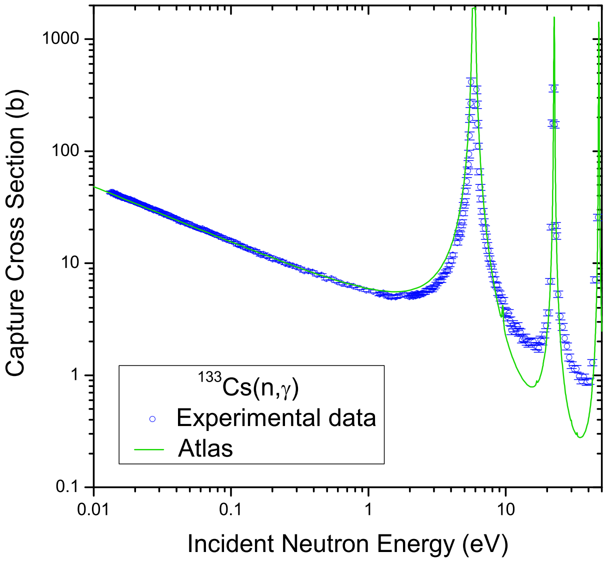

Fig. 1. Neutron capture cross section for ^{133}Cs in the thermal and resolved resonance region.

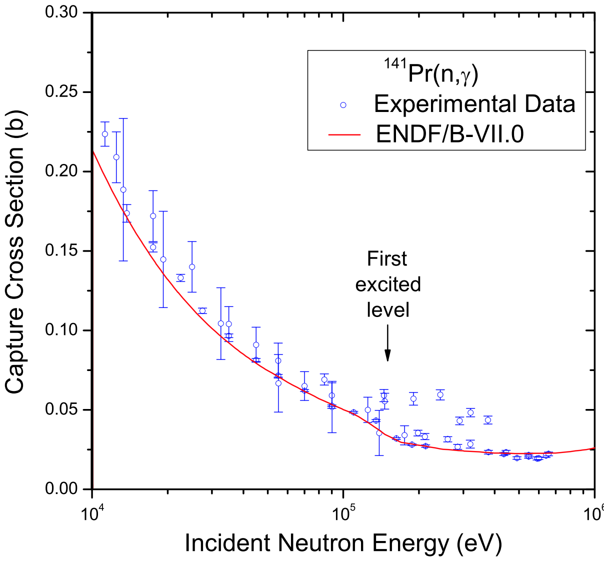

Fig. 2. Neutron capture cross section for ^{141}Pr in the unresolved resonance region extended up to the first excited level.

2.2 Fast neutron region

All evaluations in the fast neutron region were performed with the new EMPIRE code [3] that has been used for the first time to provide a number of consistent, complete evaluations to the evaluated nuclear data library. EMPIRE calculates cross sections for all relevant reaction channels, angular distributions, exclusive and inclusive particle- and γ-spectra, double-differential cross sections, and spectra of recoils. The code observes angular momentum coupling (at least in the statistical decay part) and is, therefore, capable of detailed modeling of the γ-cascade providing γ production spectra, intensities of discrete transitions, and isomeric cross sections.

The evaluation in the fast neutron region was merged with the low energy region at 1st excited level as shown in Fig. 2. In order to match two regions in a smooth way, we usually adjusted the scattering radius, R', and inserted negative cross sections background on rare occasions. Table 2 shows the boundary energy between the unresolved resonance region and the fast neutron region.

Table 2. The boundary energies between the unresolved resonance region and the fast neutron region for 32 fission products.

Isotopes	URR limit keV	Isotopes	URR limit keV
^{95}Mo	206.3	^{144}Sm	540.0
^{101}Ru	128.4	^{147}Sm	122.05
^{103}Rh	40.1	^{148}Sm	427.0
^{105}Pd	283.2	^{149}Sm	22.66
^{109}Ag	88.8	^{150}Sm	336.11
^{131}Xe	80.8	^{151}Sm	66.26
^{133}Cs	81.6	^{152}Sm	122.59
^{141}Pr	146.5	^{153}Sm	6.5
^{142}Nd	200.0	^{154}Sm	82.52
^{143}Nd	225.0	^{156}Dy	138.72
^{144}Nd	250.0	^{158}Dy	99.55
^{145}Nd	67.69	^{160}Dy	87.34
^{146}Nd	456.97	^{161}Dy	25.81
^{147}Nd	50.3	^{162}Dy	81.16
^{148}Nd	300.0	^{163}Dy	73.90
^{150}Nd	130.97	^{164}Dy	73.84

2.3 Evaluation of complete isotopic chains

A new feature of our evaluation work is a simultaneous evaluation of the complete isotopic chains for a given element. This is possible due to tremendous progress in the development of evaluation tools in recent years. The combined capabilities of the Atlas of Neutron Resonances [2], the nuclear reaction model code EMPIRE [3], input parameter libraries such as the Reference Input Parameter Library, RIPL-2 [4], experimental cross section library CSISRS/EXFOR [5], and numerous ENDF formatting and checking utilities has facilitated such a complex evaluation work. A considerable advantage of this approach is a full and consistent utilization of data that are often measured on natural elements rather than isotopes, a consistent application of model parameters, and comparison with data by summing up isotopic evaluations into a single elemental representation.

3 Results

We compared our new evaluations to the most recent major data libraries, JEFF-3.1 (released in 2005), JENDL-3.3 (released in 2002) and ENDF/B-VI.8 (released in 2001), and to the available experimental data. Figure 3 compares our (n,2n) cross sections of ^{103}Rh to them. Our evaluation reproduces the newer experimental data [8,9] well, that are higher than the older experimental data [10,11]. We note that ENDF/B-VI.8 is lower than other libraries and experimental data, and it shows unphysical behavior at high energies, due to neglect of the (n,3n) reaction channel. The capture cross sections for ^{141}Pr are compared to recent libraries and measurements as shown in Fig. 4. Our results reproduce the experimental data [12–14] around and below URR, and the experimental data [15–18] above URR.

For three isotopic chains (Nd, Sm, and Dy), we illustrate advantages of the simultaneous evaluation by plotting totether evaluated cross sections for the major reaction channels. Figure 5 present our total cross sections for all neodymium isotopes and compare them with the measured data.Our evaluations reproduce experimental data well. The only exceptions are two points by Wisshak for ^{148}Nd which appear to be suspiciously high. Our results are also in good agreement with the measured total cross section on ^{nat}Nd as shown in Fig. 6. In this case, the calculated cross sections for natural element were obtained as a sum of cross sections for all individual isotopes weighted by their respective abundances. Figure 7 shows a full set of (n,2n) cross sections for all samarium isotopes. The (n,2n) cross sections of ^{144,148,150,152,154}Sm have the experimental data, and our (n,2n) cross sections reproduce them well. Figure 8 shows the capture cross sections of all dysprosium isotopes compared to experimental data.

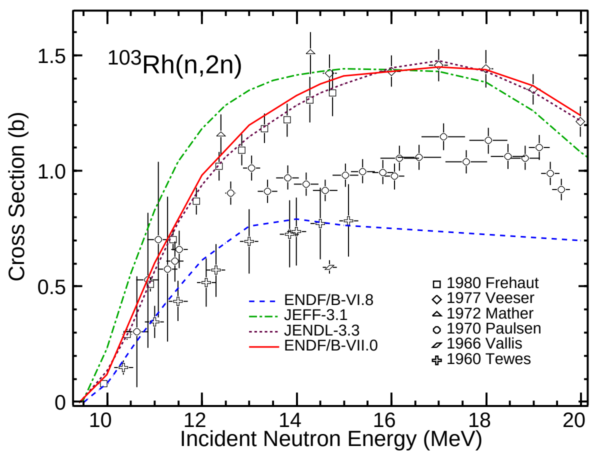

Fig. 3. Evaluated (n,2n) cross sections for ^{103}Rh compared to the ENDF/B-VI.8, JEFF-3.1 and JENDL-3.3 evaluations and to the measurements.

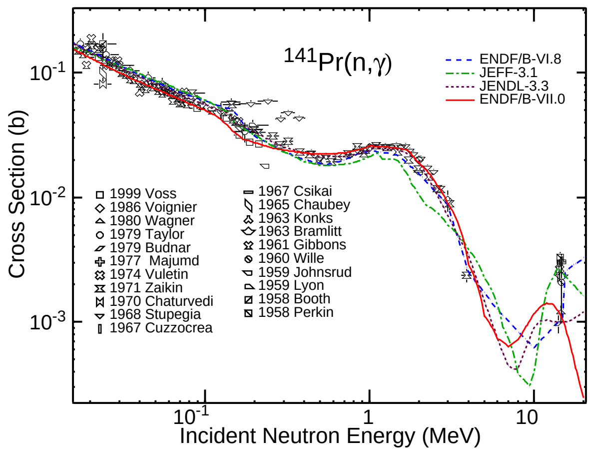

Fig. 4. Evaluated (n,γ) cross sections for ^{141}Pr in the fast neutron energy region compared to the ENDF/B-VI.8, JEFF-3.1 and JENDL-3.3 evaluations and to the measurements.

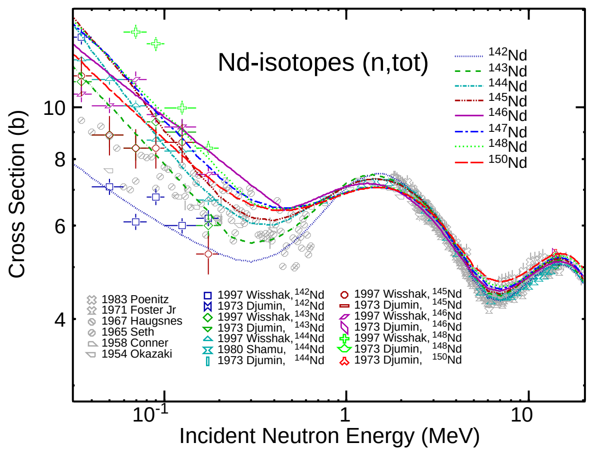

Fig. 5. Total cross sections for all neodymium isotopes compared to the measurements.

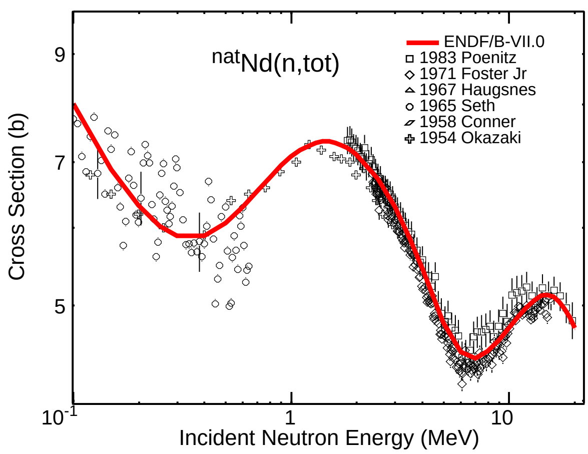

Fig. 6. Calculated total cross sections for ^{nat}Nd compared to the measurements.

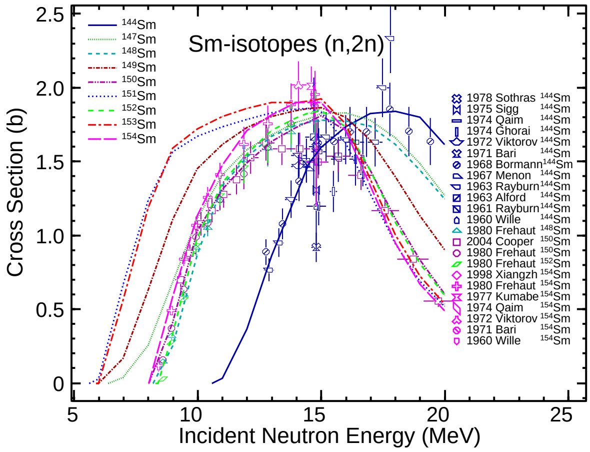

Fig. 7. (n,2n) cross sections for all samarium isotopes compared to the measurements.

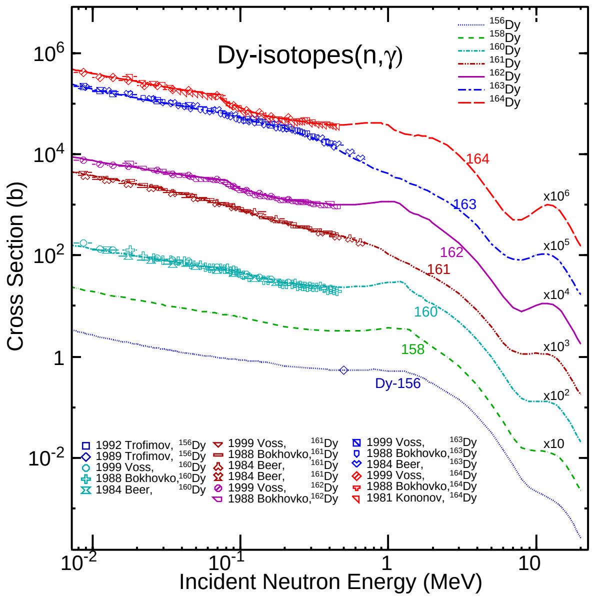

Fig. 8. Capture cross sections for all dysprosium isotopes compared to the measurements.

4 Conclusions

Neutron cross sections for 32 fission products were evaluated in the neutron-incident energy range from 10^{-5} eV to 20 MeV under the KAERI-BNL collaboration. The list of fission products consists of the priority materials for several applications, extended to cover complete isotopic chains for several elements. The full list includes 8 individual isotopes, ^{95}Mo, ^{101} Ru, ^{103}Rh, ^{105}Pd, ^{109}Ag, ^{131}Xe, ^{133}Cs, ^{141}Pr, and 24 isotopes in complete isotopic chains for Nd (8), Sm (9) and Dy (7). The evaluated data were converted into ENDF-6 formatted files, checked by a set of the CSEWG checking codes, processed with the code NJOY-99.161, and subjected to test runs with the code MCNP5 to ensure that the files can be used in transport calculations. All evaluations were adopted by the new U.S. evaluated library, ENDF/B-VII.0, released in December 2006.

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